# Fumaric acid, 3,3-dimethylbut-2-yl nonadecyl ester

**Inchi:** InChI=1S/C29H54O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-32-27(30)
**InchiKey:** AMOCDQDWTBOODW-WCWDXBQESA-N
**Formula:** C29H54O4
**SMILES:** CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
**Mol. weight [g/mol]:** 466.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -193.92 | kJ/mol | Joback Method |
| hf | -1028.30 | kJ/mol | Joback Method |
| hfus | 65.70 | kJ/mol | Joback Method |
| hvap | 96.73 | kJ/mol | Joback Method |
| log10ws | -9.41 | | Crippen Method |
| logp | 8.715 | | Crippen Method |
| mcvol | 430.050 | ml/mol | McGowan Method |
| pc | 681.36 | kPa | Joback Method |
| rinpol | 3147.00 | | NIST Webbook |
| rinpol | 3147.00 | | NIST Webbook |
| tb | 1015.99 | K | Joback Method |
| tc | 1255.41 | K | Joback Method |
| tf | 543.25 | K | Joback Method |
| vc | 1.671 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1511.33 | J/mol×K | 1015.99 | Joback Method |
| cpg | 1533.54 | J/mol×K | 1055.89 | Joback Method |
| cpg | 1554.09 | J/mol×K | 1095.80 | Joback Method |
| cpg | 1573.09 | J/mol×K | 1135.70 | Joback Method |
| cpg | 1590.67 | J/mol×K | 1175.60 | Joback Method |
| cpg | 1606.96 | J/mol×K | 1215.51 | Joback Method |
| cpg | 1622.07 | J/mol×K | 1255.41 | Joback Method |
| dvisc | 0.0002554 | Pa×s | 543.25 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000997 | Pa×s | 622.04 | Joback Method |
| dvisc | 0.0000481 | Pa×s | 700.83 | Joback Method |
| dvisc | 0.0000269 | Pa×s | 779.62 | Joback Method |
| dvisc | 0.0000167 | Pa×s | 858.41 | Joback Method |
| dvisc | 0.0000113 | Pa×s | 937.20 | Joback Method |
| dvisc | 0.0000081 | Pa×s | 1015.99 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348718&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |